\*\*\*\*\* OUERY RESULTS \*\*\*\*\*

=> d his 115

(FILE 'REGISTRY' ENTERED AT 08:13:58 ON 06 MAR 2009) SAVE TEMP L14 DAV627REGL12/A

FILE 'HCAPLUS' ENTERED AT 08:20:42 ON 06 MAR 2009

=> d que 115

L1 STR

Structure attributes must be viewed using STN Express query preparation:

Uploading L2.str

chain nodes:
8 9 11 12 14 15
ring nodes:
1 2 3 4 5 6
chain bonds:
4-11 5-8 8-9 9-14 11-12 14-15
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds:
4-11 9-14 11-12 14-15
exact bonds:
5-8 8-9
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems : containing 1 :

G1:0,S,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:CLASS

14:CLASS 15:Atom Generic attributes :

15:

Saturation : Unsaturated

Element Count : Node 12: Limited C,C1-8

L2 ( 15347) SEA FILE=REGISTRY SSS FUL L1 L3 STR

Structure attributes must be viewed using STN Express query preparation: Uploading L3.str

chain nodes : 8 9 11 12 13 14 ring nodes : 1 2 3 4 5 6 chain bonds :

```
3-13 5-8 8-9 9-11 11-12 13-14 ring bonds:  
1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds:  
3-13 9-11 11-12 13-14 exact bonds:  
5-8 8-9 normalized bonds:  
1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems:  
containing 1:
```

G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes:
12:
Saturation: Unsaturated

Element Count : Node 14: Limited C.C1-8

L4 (

G1 O.S.N

22405) SEA FILE=REGISTRY SSS FUL L3

Structure attributes must be viewed using STN Express query preparation:

chain nodes : 8 9 11 12 13 14

```
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0,S,N
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
Saturation
                    : Unsaturated
```

Element Count : Node 14: Limited C,C1-8

Structure attributes must be viewed using STN Express query preparation:

Page 4 of 49

```
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0,S,N
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
                     : Unsaturated
Saturation
Element Count :
Node 14: Limited
   C, C1-8
```

Structure attributes must be viewed using STN Express query preparation:

Page 5 of 49

```
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0,S,N
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
Saturation : Unsaturated
Element Count :
Node 14: Limited
  C,C1-8
L10 (
        5008) SEA FILE=REGISTRY SSS FUL L8 OR L9
        55683 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L4 OR L7 OR L10
L11
L12
              STR
```

Structure attributes must be viewed using STN Express query preparation: Uploading L12.str

Ak1

G2 H, [@4]

chain nodes : 8 9 10 11 13 14 15 16 17 18 19 20 27 30 31 ring nodes : 1 2 3 4 5 6 chain bonds : 5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 exact bonds : 5-8 18-19 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

```
G1:[*1],[*2],[*3]
G2:H,[*4]
Connectivity:
14:1 E exact RC ring/chain 17:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
27:CLASS 28:Atom
30:CLASS 31:CLASS
Generic attributes :
11:
                     : Unsaturated
Saturation
Element Count :
Node 11: Limited
   C, C5-10
   S.S1
Node 14: Limited
   C, C3-8
Node 17: Limited
   C, C1-3
T.14
           12 SEA FILE=REGISTRY SUB=L11 SSS FUL L12
L15
            0 SEA FILE=HCAPLUS ABB=ON PLU=ON L14
=> d his 114
    (FILE 'REGISTRY' ENTERED AT 08:13:58 ON 06 MAR 2009)
           12 S L12 FUL SUB=L11
L14
=> d que 114
L1
               STR
    Ak
```

Structure attributes must be viewed using STN Express query preparation:

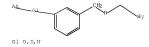
G1 0, S, N

```
chain nodes :
8 9 11 12 14 15
ring nodes :
1 2 3 4 5 6
chain bonds :
4-11 5-8 8-9 9-14 11-12 14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-11 9-14 11-12 14-15
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0,S,N
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS
14:CLASS 15:Atom
Generic attributes :
15:
Saturation
                    : Unsaturated
Element Count :
Node 12: Limited
   C,C1-8
```

L2 ( 15347) SEA FILE=REGISTRY SSS FUL L1

STR

L3



Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str

chain nodes : 8 9 11 12 13 14 ring nodes : 1 2 3 4 5 6 chain bonds : 3-13 5-8 8-9 9-11 11-12 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 3-13 9-11 11-12 13-14 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

G1:0,S,N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS Generic attributes: 12:

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8

```
L4 ( 22405)SEA FILE=REGISTRY SSS FUL L3
L5 SCR 2043 OR 1918
L6 STR
```

Structure attributes must be viewed using STN Express query preparation:

```
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
```

G1:0,S,N

```
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes:
12:
Saturation: Unsaturated
```

Page 11 of 49

Element Count : Node 14: Limited C,C1-8

Structure attributes must be viewed using STN Express query preparation:

isolated ring systems : containing 1 :

G1:0, S, N

2-13 9-11 11-12 13-14 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 6eneric attributes: 12:

Saturation

G1 0, S, N

: Unsaturated

Element Count : Node 14: Limited C,C1-8

L9 STR

Structure attributes must be viewed using STN Express query preparation:

chain nodes : 8 9 11 12 13 14 ring nodes : 1 2 3 4 5 6 chain bonds : 2-13 5-8 8-9 9-11 11-12 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 2-13 9-11 11-12 13-14 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

G1:0, S, N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS

Generic attributes : 12:

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8

L10 ( 5008) SEA FILE=REGISTRY SSS FUL L8 OR L9 L11

55683 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L4 OR L7 OR L10 L12

STR

Structure attributes must be viewed using STN Express query preparation: Uploading L12.str

chain nodes :

Page 14 of 49

```
8 9 10 11 13 14 15 16 17 18 19 20 27 30 31
ring nodes :
1 2 3 4 5 6
chain bonds :
5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20
exact bonds :
5-8 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1:
G1:[*1],[*2],[*3]
G2:H, [*4]
Connectivity:
14:1 E exact RC ring/chain 17:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
27:CLASS 28:Atom
30:CLASS 31:CLASS
Generic attributes :
11:
Saturation
                    : Unsaturated
Element Count :
Node 11: Limited
   C, C5-10
   S,S1
Node 14: Limited
   C, C3-8
Node 17: Limited
   C,C1-3
L14
          12 SEA FILE-REGISTRY SUB-L11 SSS FUL L12
=> d 114 1-12 ide
L14 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN
RN 1090692-25-3 REGISTRY
ED Entered STN: 28 Dec 2008
CN INDEX NAME NOT YET ASSIGNED
MF C24 H26 N4 O2 S
```

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SR Chemical Library Supplier: Ambinter LC STN Files: CHEMCATS

$$\begin{array}{c} \text{Ph-} \text{CH}_2 - \text{O} \\ \\ \end{array} \begin{array}{c} \text{Et} \\ \text{CH}_2 - \text{h-} \text{CH}_2 \\ \end{array} \begin{array}{c} \text{N} \\ \\ \end{array} \begin{array}{c} \text{S} \\ \\ \end{array} \begin{array}{c} \text{E}^{\text{I}} \\ \end{array}$$

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1089649-59-1 REGISTRY

ED Entered STN: 24 Dec 2008

CN INDEX NAME NOT YET ASSIGNED

MF C23 H24 N4 O3 S

SR Chemical Library

Supplier: Ambinter LC STN Files: CHEMCATS

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1030752-95-4 REGISTRY

ED Entered STN: 26 Jun 2008

CN Thieno[2,3-d]pyrimidine-2-methanamine, 4-amino-N,5,6-trimethyl-N-[[4-(2-propen-1-yloxy)phenyl]methyl]- (CA INDEX NAME)

MF C20 H24 N4 O S

SR Chemical Library

Supplier: Aurora Fine Chemicals

LC STN Files: CHEMCATS

Page 16 of 49

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1013727-14-4 REGISTRY

ED Entered STN: 11 Apr 2008

CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5-(4-fluorophenyl)-2-[[methyl[[4-(2-

propen-1-yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)

MF C24 H22 F N3 O2 S SR

Chemical Library

Supplier: Ambinter LC STN Files: CHEMCATS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1013599-48-8 REGISTRY

ED Entered STN: 10 Apr 2008

CN Thieno[2,3-d]pyrimidine-6-carboxylic acid, 1,4-dihydro-5-methyl-2-[[methyl[[4-(2-propen-1yloxy)phenyl]methyl]amino]methyl]-4-oxo-, 2-methoxyethyl ester (CA INDEX NAME)

MF C23 H27 N3 O5 S

SR Chemical Library Supplier: Ambinter

LC STN Files: CHEMCATS

$$\begin{array}{c} \text{H}_2\text{C} = \text{CH}_2 - \text{CH}_$$

PAGE 1-B

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1013300-64-5 REGISTRY

ED Entered STN: 10 Apr 2008

CN Thieno[2,3-d]pyrimidin-4(1H)-one, 5-(2-chlorophenyl)-2-[[methyl[[4-(2-

propen-1-yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)

MF C24 H22 C1 N3 O2 S

SR Chemical Library

Supplier: Ambinter LC STN Files: CHEMCATS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 949406-17-1 REGISTRY

ED Entered STN: 05 Oct 2007

CN Thieno[3,2-d]pyrimidin-4(3H)-one, 2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)

MF C18 H19 N3 O2 S

SR Chemical Library

Supplier: Enamine

LC STN Files: CHEMCATS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 930905-89-8 REGISTRY

ED Entered STN: 19 Apr 2007

CN Thieno[2,3-d]pyrimidine-6-carboxylic acid,

4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-, ethyl ester (CA INDEX NAME)

MF C22 H26 N4 O3 S

SR Chemical Library

Supplier: Enamine

LC STN Files: CHEMCATS

$$\begin{array}{c} \text{H2C} = \text{CH} - \text{CH}_2 - \text{O} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{He} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 930016-76-5 REGISTRY

ED Entered STN: 13 Apr 2007

CN Thieno[3,2-d]pyrimidin-4(3H)-one, 2-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]- (CA INDEX NAME)

MF C23 H23 N3 O3 S

SR Chemical Library

Supplier: Enamine

LC STN Files: CHEMCATS

- \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*
- L14 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN
- RN 924238-94-8 REGISTRY
- ED Entered STN: 02 Mar 2007
- CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,
  7-[[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]methylamino]methyl]- (CA
  INDEX NAME)
- MF C23 H23 N3 O3 S
- SR Chemical Library

Supplier: Aurora Fine Chemicals

LC STN Files: CHEMCATS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN

RN 876579-73-6 REGISTRY

ED Entered STN: 13 Mar 2006

CN 4H-Cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one,

1,5,6,7-tetrahydro-2-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 4H-Cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one, 1,5,6,7-tetrahydro-2-[[methyl[[4-(2-propenyloxy)phenyl]methyl]amino]methyl]- (9CI)

MF C21 H23 N3 O2 S SR Chemical Library

Supplier: Aurora Fine Chemicals

LC STN Files: CHEMCATS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L14 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2009 ACS on STN
- RN 871092-29-4 REGISTRY
- ED Entered STN: 04 Jan 2006
- CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[methyl[[4-(2-propen-1-yloxy)phenyl]methyl]amino]methyl]-3-phenyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

- CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,
  - 7-[[methyl][4-(2-propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl- (9CI)
- MF C24 H23 N3 O2 S
- SR Chemical Library
- Supplier: Enamine
- LC STN Files: CHEMCATS

$$\begin{array}{c} \text{H}_2\text{C} = \text{CH} - \text{CH}_2 - \text{O} \\ \\ \text{CH}_2 - \text{II} - \text{CH}_2 - \text{II} \\ \\ \end{array} \begin{array}{c} \text{S} \\ \text{Pt} \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

=> d his 116

(FILE 'REGISTRY' ENTERED AT 08:21:32 ON 06 MAR 2009)
FILE 'CHEMCATS' ENTERED AT 08:58:39 ON 06 MAR 2009

L16 30 S L14

FILE 'REGISTRY' ENTERED AT 09:01:42 ON 06 MAR 2009

FILE 'CHEMCATS' ENTERED AT 09:01:45 ON 06 MAR 2009

=> d que 116 L1 STR

Structure attributes must be viewed using STN Express query preparation: Uploading L2.str

3 14 15

chain nodes:
8 9 11 12 14 15
ring nodes:
1 2 3 4 5 6
chain bonds:
4-11 5-8 8-9 9-14 11-12 14-15
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds:

4-11 9-14 11-12 14-15 exact bonds: 5-8 8-9 normalized bonds: 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems: containing 1:

G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:CLASS 14:CLASS 15:Atom Generic attributes:
15:

: Unsaturated

Element Count : Node 12: Limited C,C1-8

Saturation

Structure attributes must be viewed using STN Express query preparation: Uploading  $L3.\mathrm{str}$ 

chain nodes :

```
8 9 11 12 13 14 ring nodes:
1 2 3 4 5 6 chain bonds:
3-13 5-8 8-9 9-11 11-12 13-14 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds:
3-13 9-11 11-12 13-14 exact bonds:
5-8 8-9 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems: containing 1:
```

G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes:

12: Saturation

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8

Structure attributes must be viewed using STN Express query preparation:

Uploading L5.str

```
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
```

G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 4:CLASS
Generic attributes:
12:

12:

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8

L7 ( 
$$26302$$
)SEA FILE=REGISTRY SSS FUL L6 NOT L5 L8 STR

Structure attributes must be viewed using STN Express query preparation:

chain nodes : 8 9 11 12 13 14 ring nodes : 1 2 3 4 5 6 chain bonds : 2-13 5-8 8-9 9-11 11-12 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 2-13 9-11 11-12 13-14 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

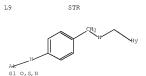
G1:0,S,N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS Generic attributes:

Generic attributes : 12:

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8



Structure attributes must be viewed using STN Express query preparation:

```
Uploading L7.str
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1:
G1:0,S,N
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
Saturation
                    : Unsaturated
Element Count :
Node 14: Limited
   C, C1-8
```

```
L10 ( 5008)SEA FILE=REGISTRY SSS FUL L8 OR L9
L11 55683 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L4 OR L7 OR L10
L12 STR
```

Ak1

Structure attributes must be viewed using STN Express query preparation: Uploading L12.str

chain nodes : 8 9 10 11 13 14 15 16 17 18 19 20 27 30 31 ring nodes : 1 2 3 4 5 6 chain bonds : 5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 exact bonds : 5-8 18-19 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

```
G1:[*1],[*2],[*3]
G2:H,[*4]
Connectivity:
14:1 E exact RC ring/chain 17:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
27:CLASS 28:Atom
30:CLASS 31:CLASS
Generic attributes :
11:
Saturation
               : Unsaturated
Element Count :
Node 11: Limited
   C, C5-10
    S,S1
Node 14: Limited
   C, C3-8
Node 17: Limited
   C.C1-3
           12 SEA FILE=REGISTRY SUB=L11 SSS FUL L12
T.14
L16
            30 SEA FILE=CHEMCATS ABB=ON PLU=ON L14
=> fil stng
FILE 'STNGUIDE' ENTERED AT 09:02:05 ON 06 MAR 2009
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 27, 2009 (20090227/UP).
=> d 116 1-30 ide
L16 ANSWER 1 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN
Accession No. (AN): 2061673348 CHEMCATS
                  (CO): Ambinter Stock Screening Collection
Catalog Name
Publication Date
                  (PD): 21 Nov 2008
Order Number
                  (ON): T6055864
Chemical Name
                   (CN): Thieno[2,3-d]pyrimidine-2-methanamine,
                         4-amino-N, 5, 6-trimethyl-N-[[4-(2-propen-1-
                         vloxy)phenyl]methyl]-
CAS Registry No. (RN): 1030752-95-4
Supplementary Term (ST): CHEMICAL LIBRARY
Structure
                      :
```

L16 ANSWER 2 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2061042000 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

(PD): 21 Nov 2008 Publication Date

Order Number (ON): T6216377

(CN): Chemical name not vet assigned Chemical Name

CAS Registry No. (RN): 1089649-59-1

Supplementary Term (ST): CHEMICAL LIBRARY :

Structure

L16 ANSWER 3 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2060875760 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

(PD): 21 Nov 2008 Publication Date

Order Number (ON): T5954092

Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one, 2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-

CAS Registry No. (RN): 949406-17-1

Structure

Supplementary Term (ST): CHEMICAL LIBRARY

L16 ANSWER 4 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN Accession No. (AN): 2060671762 CHEMCATS

(CO): Ambinter Stock Screening Collection Catalog Name

Publication Date (PD): 21 Nov 2008 Order Number (ON): T6261100

Chemical Name (CN): Chemical name not yet assigned

CAS Registry No. (RN): 1090692-25-3 Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L16 ANSWER 5 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2060237217 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

Publication Date (PD): 21 Nov 2008

Order Number (ON): T5833544

Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,

4-amino-5-methyl-2-[[methyl[[4-(2-propen-1yloxy)phenyl]methyl]amino]methyl]-, ethyl ester

CAS Registry No. (RN): 930905-89-8

Supplementary Term (ST): CHEMICAL LIBRARY :

Structure

H2C CH CH2-

L16 ANSWER 6 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

(AN): 2060226305 CHEMCATS Accession No.

Catalog Name (CO): Ambinter Stock Screening Collection

(PD): 21 Nov 2008 Publication Date

Order Number (ON): T5810150

(CN): Thieno[3,2-d]pyrimidin-4(3H)-one, Chemical Name

2-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]-

CAS Registry No. (RN): 930016-76-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L16 ANSWER 7 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2060163673 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

Publication Date (PD): 21 Nov 2008 Order Number (ON): T5682113

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]-

CAS Registry No. (RN): 924238-94-8

Supplementary Term (ST): CHEMICAL LIBRARY Structure :

L16 ANSWER 8 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2056291684 CHEMCATS
Catalog Name (CO): AKos Screening Library

Publication Date (PD): 18 Jul 2008 Order Number (ON): AKE-PB65201304

Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,

5-(4-fluorophenyl)-2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-

CAS Registry No. (RN): 1013727-14-4 Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

L16 ANSWER 9 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

(AN): 2055673608 CHEMCATS Accession No. Catalog Name (CO): AKos Screening Library

(PD): 18 Jul 2008 Publication Date

Order Number (ON): AKE-PB-12658864

Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,

1,4-dihydro-5-methyl-2-[[methyl[[4-(2-propen-1yloxy)phenyl]methyl]amino]methyl]-4-oxo-,

2-methoxvethvl ester

CAS Registry No. (RN): 1013599-48-8

Supplementary Term (ST): CHEMICAL LIBRARY; CHEMICAL LIBRARY

Structure

H2C == CH = CH2 = O.

PAGE 1-B

— ОМе

L16 ANSWER 10 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2055659677 CHEMCATS

Catalog Name (CO): AKos Screening Library Publication Date (PD): 18 Jul 2008

Order Number (ON): AKE-PB-12658896

Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,

5-(2-chlorophenyl)-2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-

CAS Registry No. (RN): 1013300-64-5

Supplementary Term (ST): CHEMICAL LIBRARY; CHEMICAL LIBRARY

Structure :

H2C CH CH2 - O.

L16 ANSWER 11 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2049271778 CHEMCATS
Catalog Name (CO): Aurora Screening Library

Publication Date (PD): 13 Jun 2008

Order Number (ON): ken-533977

Chemical Name (CN): Thieno[2,3-d]pyrimidine-2-methanamine, 4-amino-N,5,6-trimethyl-N-[[4-(2-propen-1-

yloxy)phenyl]methyl]-

CAS Registry No. (RN): 1030752-95-4 Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

L16 ANSWER 12 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048987769 CHEMCATS
Catalog Name (CO): Aurora Screening Library

Publication Date (PD): 13 Jun 2008

Order Number (ON): kuk-524975

Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,

5-(4-fluorophenyl)-2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-

CAS Registry No. (RN): 1013727-14-4 Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

L16 ANSWER 13 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048982718 CHEMCATS

Catalog Name (CO): Aurora Screening Library

Publication Date (PD): 13 Jun 2008 Order Number (ON): kuk-420081

Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid, 1,4-dihydro-5-methyl-2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-4-oxo-,

2-methoxvethvl ester

CAS Registry No. (RN): 1013599-48-8

Supplementary Term (ST): CHEMICAL LIBRARY .

Structure

PAGE 1-A

$$\label{eq:h2C} \begin{array}{c} \text{H}_2\text{C} = \text{CH}_2\text{-CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{CH}_2 - \text{I}_{\text{L}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{Me} \end{array}$$

PAGE 1-B

— ОМе

L16 ANSWER 14 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048968843 CHEMCATS

Catalog Name (CO): Aurora Screening Library (PD): 13 Jun 2008 Publication Date

Order Number (ON): kuk-420083

Chemical Name (CN): Thieno[2,3-d]pyrimidin-4(1H)-one,

5-(2-chlorophenv1)-2-[[methv1][4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-

CAS Registry No. (RN): 1013300-64-5

Supplementary Term (ST): CHEMICAL LIBRARY Structure :

L16 ANSWER 15 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

(AN): 2048606252 CHEMCATS Accession No.

Catalog Name (CO): Aurora Screening Library

(PD): 13 Jun 2008 Publication Date

Order Number (ON): ken-374837

Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,

2-[[methy1[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-(RN): 949406-17-1 CAS Registry No.

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

L16 ANSWER 16 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048515080 CHEMCATS (CO): Aurora Screening Library

Catalog Name Publication Date (PD): 13 Jun 2008

Order Number (ON): ken-268646

Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-5-methyl-2-[[methyl[[4-(2-propen-1yloxy)phenyl]methyl]amino]methyl]-, ethyl ester

CAS Registry No. (RN): 930905-89-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

$$\begin{array}{c} \text{H}_2\text{C} = \text{CH} - \text{CH}_2 - \text{O} \\ \text{CH}_2 - \text{IL} - \text{CH}_2 - \text{IL} \\ \text{OET} \end{array}$$

L16 ANSWER 17 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2048475470 CHEMCATS

Catalog Name (CO): Aurora Screening Library Publication Date (PD): 13 Jun 2008

Order Number (ON): ken-248130

Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,

2-[[[[3-methoxy-4-

(phenylmethoxy)phenyllmethyllmethylaminolmethyll-

CAS Registry No. (RN): 930016-76-5 Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L16 ANSWER 18 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2044099010 CHEMCATS

Catalog Name (CO): Ryan Scientific Screening Library

(PD): 25 Jan 2008 Publication Date Order Number (ON): T5810150

Chemical Name (CN): Thieno[3,2-d]pvrimidin-4(3H)-one,

2-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]-

CAS Registry No. (RN): 930016-76-5

Supplementary Term (ST): CHEMICAL LIBRARY Structure :

L16 ANSWER 19 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2044006130 CHEMCATS

Catalog Name (CO): Ryan Scientific Screening Library

(PD): 25 Jan 2008 Publication Date

Order Number (ON): T5435667

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[methyl[[4-(2-

propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl-(RN): 871092-29-4

CAS Registry No.

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

$$\begin{array}{c} \text{H2C} = \text{CH} - \text{CH2} - 0 \\ \text{CH2} - \text{H} - \text{CH2} - \text{H} \\ \text{CH2} - \text{H} - \text{CH2} \end{array}$$

L16 ANSWER 20 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2042694057 CHEMCATS

Catalog Name (CO): Ryan Scientific Screening Library

Publication Date (PD): 25 Jan 2008

Order Number (ON): T5833544

Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid, 4-amino-5-methyl-2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-, ethyl ester

CAS Registry No. (RN): 930905-89-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L16 ANSWER 21 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2042635941 CHEMCATS

Catalog Name (CO): Ryan Scientific Screening Library

Publication Date (PD): 25 Jan 2008 Order Number (ON): T5682113

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]-

CAS Registry No. (RN): 924238-94-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L16 ANSWER 22 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2039512617 CHEMCATS
Catalog Name (CO): Enamine Screening Library

Publication Date (PD): 17 Jan 2008

(ON): T5954092 Order Number

Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one, 2-[[methyl[[4-(2-propen-1-

yloxy)phenyl]methyl]amino]methyl]-CAS Registry No. (RN): 949406-17-1

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

H2C==CH=CH2=C

L16 ANSWER 23 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2037934481 CHEMCATS

Catalog Name (CO): Aurora Screening Library

Publication Date (PD): 13 Jun 2008

Order Number (ON): ken-092588

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]-

CAS Registry No. (RN): 924238-94-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure .

L16 ANSWER 24 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

(AN): 2033762283 CHEMCATS Accession No.

Catalog Name (CO): Enamine Screening Library

Publication Date (PD): 17 Jan 2008 Order Number (ON): T5833544

Chemical Name (CN): Thieno[2,3-d]pyrimidine-6-carboxylic acid,

4-amino-5-methyl-2-[[methyl[[4-(2-propen-1yloxy)phenyl]methyl]amino]methyl]-, ethyl ester

CAS Registry No. (RN): 930905-89-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

$$\begin{array}{c} \text{H}_2\text{C} = \text{CH}_2 - \text{CH}_2 - \text{O} \\ \text{CH}_2 - \text{H}_2 - \text{CH}_2 - \text{H}_2 \\ \text{H}_{12} \end{array} \\ \begin{array}{c} \text{OBt} \\ \text{H}_{12} \end{array}$$

L16 ANSWER 25 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2033646191 CHEMCATS

Catalog Name (CO): Enamine Screening Library

Publication Date (PD): 17 Jan 2008 Order Number (ON): T5682113

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[[[3-methoxy-4-

(phenylmethoxy)phenyl]methyl]methylamino]methyl]-

CAS Registry No. (RN): 924238-94-8

Supplementary Term (ST): CHEMICAL LIBRARY :

Structure

L16 ANSWER 26 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2033572764 CHEMCATS Catalog Name

(CO): Enamine Screening Library

Publication Date (PD): 17 Jan 2008 Order Number (ON): T5810150

Chemical Name (CN): Thieno[3,2-d]pyrimidin-4(3H)-one,

2-[[[3-methoxy-4-

(phenylmethoxy)phenyllmethyllmethylaminolmethyll-

CAS Registry No. (RN): 930016-76-5 Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L16 ANSWER 27 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2029314936 CHEMCATS

Catalog Name (CO): Aurora Screening Library

Publication Date (PD): 13 Jun 2008 Order Number (ON): kend-0120483

Chemical Name (CN): 4H-Cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one,

1,5,6,7-tetrahydro-2-[[methyl[[4-(2propenyloxy)phenyl]methyl]amino]methyl]-

CAS Registry No. (RN): 876579-73-6 Supplementary Term (ST): CHEMICAL LIBRARY

Supplementary Term (ST): CHEMICAL LIB Structure :

L16 ANSWER 28 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2028893097 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

Publication Date (PD): 21 Nov 2008 Order Number (ON): T5435667

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[methy1[[4-(2-

propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl-CAS Registry No. (RN): 871092-29-4

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

H<sub>2</sub>C=CH-CH<sub>2</sub>-0 Me CH<sub>2</sub>-1 CH<sub>2</sub>-1 CH<sub>2</sub>-1 S

L16 ANSWER 29 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2026298900 CHEMCATS
Catalog Name (CO): Aurora Screening Library

Publication Date (PD): 13 Jun 2008

Order Number (ON): kenc-0030177

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,

7-[[methyl[[4-(2-

propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl-

CAS Registry No. (RN): 871092-29-4

Supplementary Term (ST): CHEMICAL LIBRARY Structure :

$$\begin{array}{c} \text{H2C} = \text{CH} - \text{CH2} - \text{O} \\ \text{CH2} - \text{H2} - \text{CH2} \\ \end{array}$$

L16 ANSWER 30 OF 30 CHEMCATS COPYRIGHT 2009 ACS on STN

Accession No. (AN): 2025394232 CHEMCATS

Catalog Name (CO): Enamine Screening Library

Publication Date (PD): 17 Jan 2008 Order Number (ON): T5435667

Chemical Name (CN): 5H-Thiazolo[3,2-a]pyrimidin-5-one,
7-[[methyl][4-(2-

propenyloxy)phenyl]methyl]amino]methyl]-3-phenyl-

CAS Registry No. (RN): 871092-29-4

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

$$\begin{array}{c} \text{H2C} = \text{CH} - \text{CH2} - \text{O} \\ \text{CH2} - \text{In} - \text{CH2} - \text{In} \\ \text{CH2} - \text{In} - \text{CH2} - \text{In} \\ \end{array}$$

# \*\*\*\*\* SEARCH HISTORY \*\*\*\*\*

=> d his nofi

(FILE 'HOME' ENTERED AT 08:13:30 ON 06 MAR 2009)

FILE 'REGISTRY' ENTERED AT 08:13:58 ON 06 MAR 2009 ACT DAV627MAIN/A

-----

L1 STR

Uploading L2.str

11

chain nodes : 8 9 11 12 14 15 ring nodes : 1 2 3 4 5 6 chain bonds : 4-11 5-8 8-9 9-14 11-12 14-15 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 4-11 9-14 11-12 14-15 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

G1:0,S,N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:CLASS 14:CLASS 15:Atom

Generic attributes : 15:

Saturation : Unsaturated

Element Count : Node 12: Limited C,C1-8 L2 ( 15347) SEA SSS FUL L1 L3 STR

Uploading L3.str

chain nodes : 8 9 11 12 13 14 ring nodes : 1 2 3 4 5 6 chain bonds : 3-13 5-8 8-9 9-11 11-12 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 3-13 9-11 11-12 13-14 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

G1:0,S,N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS Generic attributes:

12:

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8 L5 SCR 2043 OR 1918 L6 STR

Uploading L5.str

CH<sub>2</sub> N

chain nodes : 8 9 11 12 13 14 ring nodes : 1 2 3 4 5 6 chain bonds : 2-13 5-8 8-9 9-11 11-12 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds : 2-13 9-11 11-12 13-14 exact bonds : 5-8 8-9 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1:

G1:0,S,N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS Generic attributes: 12:

: Unsaturated

Saturation
Element Count :
Node 14: Limited
C,C1-8

L7 ( 26302)SEA SSS FUL L6 NOT L5 L8 STR

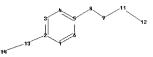
Page 45 of 49

```
chain nodes :
8 9 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
2-13 5-8 8-9 9-11 11-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
2-13 9-11 11-12 13-14
exact bonds :
5-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:0,S,N
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom
13:CLASS 14:CLASS
Generic attributes :
12:
Saturation
               : Unsaturated
Element Count :
Node 14: Limited
   C,C1-8
```

Uploading L7.str

STR

1.9



chain nodes:

8 9 11 12 13 14

ring nodes:
1 2 3 4 5 6

chain bonds:
2-13 5-8 8-9 9-11 11-12 13-14

ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds:
2-13 9-11 11-12 13-14

```
exact bonds:
5-8 8-9
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems:
containing 1:
```

G1:0.S.N

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS Generic attributes:

12:

Saturation : Unsaturated

Element Count : Node 14: Limited C,C1-8

L10 ( 5008)SEA SSS FUL L8 OR L9
L11 55683 SEA ABB=ON PLU=ON L2 OR L4 OR L7 OR L10
------L12 STRUCTURE UPLOADED

Uploading L12.str



chain nodes :
8 9 10 11 13 14 15 16 17 18 19 20 27 30 31 ring nodes :
1 2 3 4 5 6 chain bonds :
5-8 8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 18-19 ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 exact/norm bonds :
8-9 9-10 10-11 10-30 10-31 13-27 15-18 16-20 exact bonds :

```
5-8 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:[*1],[*2],[*3]
G2:H,[*4]
Connectivity:
14:1 E exact RC ring/chain 17:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
27:CLASS 28:Atom
30:CLASS 31:CLASS
Generic attributes :
Saturation
                     : Unsaturated
Element Count :
Node 11: Limited
   C, C5-10
   S,S1
Node 14: Limited
   C, C3-8
Node 17: Limited
   C.C1-3
L13
            1 SEA SUB=L11 SSS SAM L12
               D SCAN
L14
            12 SEA SUB=L11 SSS FUL L12
               SAVE TEMP L14 DAV627REGL12/A
    FILE 'HCAPLUS' ENTERED AT 08:20:42 ON 06 MAR 2009
L15
             0 SEA ABB=ON PLU=ON L14
    FILE 'CHEMCATS' ENTERED AT 08:58:39 ON 06 MAR 2009
1.16
            30 SEA ABB=ON PLU=ON L14
               D
               D OUE L15
               D OUE L14
    FILE 'REGISTRY' ENTERED AT 09:01:42 ON 06 MAR 2009
               D L14 1-12 IDE
    FILE 'CHEMCATS' ENTERED AT 09:01:45 ON 06 MAR 2009
               D OUE L16
    FILE 'STNGUIDE' ENTERED AT 09:02:05 ON 06 MAR 2009
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FILE 'CHEMCATS' ENTERED AT 09:02:14 ON 06 MAR 2009
D L16 1-30 IDE

FILE 'SINGUIDE' ENTERED AT 09:02:18 ON 06 MAR 2009